SAT Report for Case # LM-17-0030

General

[redacted]

Report Status: Complete
Status Date: 08/30/2017
CRSS Date: 08/31/2017
SAT Date: 09/01/2017
SAT Chair: [redacted]
Consolidated PMN?
Consolidated Set:
Submitter: Soulbrain MI
CAS Number: 1072-53-3
Ecotox Related Cases: [redacted]
Health Related Cases: [redacted]
Chemical Name: 1,3,2-Dioxathiolane, 2,2-dioxide
Use: [redacted]
Trade name: ESA, DTD
PV Max (kg/yr):
Ecotox Assessor: [redacted]
Fate Assessor: [redacted]
Health Assessor: [redacted]

Physical Chemical Information

Molecular Weight:	124.12	**Physical State - Neat:**	Solid		
Percent 500:		**Percent 1000:**			
Melting Point (Measured):	96.00 - 99.00	**Melting Point (est):**		**MPD (EPI):**	
Vapor Pressure:		**Vapor Pressure (est):**	0.04	**VP (EPI):**	
Water Solubility:		**Water Solubility (EST):**	382	**Water Solubility (EPI):**	
Log Kow:				**Log Kow (EPI):**	
Log P:		**Log P Comment:**			

SAT Concern

Ecotox Rating (1):	2	**Ecotox Rating Comment (1):**	PMN substance
Ecotox Rating (2):		**Ecotox Rating Comment (2):**	
Health Rating (1):	2	**Health Rating Comment (1):**	
Health Rating (2):		**Health Rating Comment (2):**	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
3	1	2	

Exposure Based Review (Health)?	N
Exposure Based Review (Ecotox)?	N
SAT Keywords:	SEVER IRR/CORR.E, S, L, SENS, ACUTE, LIVER, DEVEL, MUTA, ONCO, AQUATOX.

Fate Assessment Summary: M-17-0030

FATE:
Solid with MP = 96-99 °C (M)

log Kow = -0.90 (E)
S = 382 mg/L at 25 °C (E)
VP = 0.04 torr
at 25 °C (E)
BP = 209 °C (E)
H = 1.15E-6 (E)
log Koc = 0.97
(E)
log Fish BCF = 0.5 (3) (E)
log Fish BAF = -0.047 (0.9) (E)

POTW removal (%) = 0-25
Time for complete ultimate aerobic biodeg
= mo
Sorption to soils/sediments = low
Volatilization half-life
from a standard river = 570 hrs
Volatilization half-life from a
standard lake = 260 da
Atmospheric Oxidation Half-life = 120 hr via OH
radical
PBT Potential: P3B1
*CEB FATE: Migration to ground water =
rapid
Bioconcentration factor to be put into E-FAST: 3.2

PMN
Material:
Overall wastewater treatment removal is 0-25% due to low biodegradability, low sorption and low stripping.
Sorption to sludge
is low based on the estimated physical-chemical properties from EPISuite and analogous chemicals.

Air Stripping (Volatilization to air) is
negligible based on the estimated Henry's Law Constant.
Removal by
biodegradation in wastewater treatment is negligible based on BIOWIN model
estimates and analogous chemicals.
The aerobic aquatic biodegradation
half-life is months based on BIOWIN model estimates and analogous chemicals.
The anaerobic aquatic biodegradation half-life is greater
than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is low based on the estimated PCKOC model estimates and analogous chemicals.
Migration to groundwater is
rapid based on the estimated PCKOC model estimates and analogous chemicals.
PMN Material:
High Persistence (P3) is based on the
anaerobic biodegradation half-life and analogous chemicals.
Low
Bioaccumulation potential (B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast: BCF: 3.2
NOTE: The chemical may be inherently
biodegradable.

Removal in WWT/POTW (Overall): 0-25

Condition	Rating Values w/ Rating Description	Comment
WWT/POTW Sorption:	1	
WWT/POTW Stripping:	4	
Biodegradation Removal:	4	
Biodegradation Destruction:	3	

Condition	Rating Values w/ Rating Description	Comment
Aerobic Biodeg Ult:		
Aerobic Biodeg Prim:		
Anaerobic Biodeg Ult:	4	
Anaerobic Biodeg Prim:		
Hydrolysis (t1/2 at pH 7,25C) A:		
Hydrolysis (t1/2 at pH 7,25C) B:		
Sorption to Soils/Sediments:	4	
Migration to Ground Water:	4	
Photolysis A, Direct:		
Photolysis B, Indirect:		
Atmospheric Ox A, OH:		
Atmospheric Ox B, O3:		

Health Assessment

Health Summary: Absorption is nil through the skin as the neat material and moderate when in solution and moderate absorption through the lung and GI tract (pchem). The PMN is a potential alkylating agent. Available data suggest mutagenicity concerns and severe irritation and corrosion to eyes and skin and likely other tisssues such as mucous membrances and lung. Based on the alkylating potential of the LVE modification, there are also concerns for respiratory and dermal sensitization, acute effects, liver toxicity, developmental toxicity, and oncogenicity.

Routes of Exposure: Dermal Drinking Water
Inhalation

Test Data Submitted

Test Data Submitted: [redacted]

Ecotox Assessment

Test organism	Test Type	Test Endpoint	Predicted	Measured	Comments
Fish	96-h	LC50	> 100	[redacted]	[redacted]
Daphnid	48-h	LC50	> 100	[redacted]	" "
Green Algae	96-h	EC50	> 100	[redacted]	" "
Fish	-	Chronic Value	> 10		" "
Daphnid	-	Chronic Value	> 10		" "
Green Algae	-	Chronic Value	> 10	[redacted]	" "

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Acquatic:		5	5000	Acute/Chronic; Based on algae ChV
Chronic Acquatic:		10	500	Acute/Chronic

Ecotox Route of Exposure?	No releases to water

Factors	Values	Comments
SARs:	Esters	
SAR Class:	Esters	
TSCA NCC Category?	Esters	

Recommended Testing

Ecotox Value Comments

Predictions are based on QSARs for esters (ECOSAR V2.2); MW 124; Log Kow = -0.90 (P); solid with a MP = 99C (M); S = 382,000 mg/L (P); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.

Ecotox Factors Comments

Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model).
Based on these estimated hazard values, EPA concludes that this chemical substance has moderate environmental hazard.

· Substance falls within the TSCA New Chemicals Category of Esters.
· SAR chemical class of esters.

· Moderate hazard based on acute and chronic COCs of 5,000 and 500 ppb, respectively.

Environmental Risk:
· Risks were not identified.

Testing Recommendations:
· No testing recommended.